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Density Functional Study of the 1,4-Polymerization of Butadiene with Cationic $[Ni^{II}(C_4H_7)(C_4H_6)PH_3]^+$ Complexes.

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According to the π-allyl-insertion mechanism[1] the entire catalytic cycle of 1,4-polymerization of butadiene has been theoretically studied by employing a gradient-corrected density functional method with the cationic butenylbis(ligand) complexes as the catalyst.[2] We have investigated competitive chain propagation cycles for generation of a cis-1,4- and trans-1,4-polymer, and also anti-syn isomerization. The calculations provide a clear insight into the stereoregulation mechanism of trans-1,4 polymerization.

1 Taube, R.; Gehrke, J.-P.; Böhme, P. *Wiss. Zeitschr. TH Leuna-Merseburg* **1987**, *39*, 310.
2 Tobisch, S.; Bögel, H.; Taube, R. *Organometallics* **1998**, *17*, 1177.